Correlated hopping in infinite dimensions: Rigorous local approach

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Abstract

The general approach for the description of correlated hopping in the Dynamical Mean-Field Theory which is based on the expansion over electron hopping around the atomic limit is developed. It is formulated in terms of the local irreducible parts (cumulants) of Green's functions and allowed to calculate thermodynamical functions. As a limit case the Falicov–Kimball model with correlated hopping is considered.

The main idea of the Dynamical Mean-Field Theory (DMFT) is in the local (single-site) nature of the self-energy [1, 2]. But this statement violates for the systems with correlated hopping, when self-energy becomes unlocal [3]. In this article we present the general DMFT approach for the description of correlated hopping which is based on the expansion over electron hopping around the atomic limit [4, 5] and allows to build DMFT in terms of local quantities. As a limit case the Falicov-Kimball model with correlated hopping is considered.

In general, the hopping term of the Hamiltonian with correlated hopping for the Falicov–Kimball model can be written as

$$H_t = \frac{1}{\sqrt{D}} \sum_{<ij>} d_i^\dagger d_j \Big[t_{ij}^{++} P_i^+ P_j^+ + t_{ij}^{--} P_i^- P_j^- + t_{ij}^{+-} P_i^+ P_j^- + t_{ij}^{-+} P_i^- P_j^+ \Big], \tag{1}$$

where the projection operators $P_i^+ = n_{if}$, $P_i^- = 1 - n_{if}$ on the states of f-particles are introduced. It is convenient to rewrite it in matrix notations

$$H_t = \frac{1}{\sqrt{D}} \sum_{<ij>} \mathbf{d}_i^\dagger \mathbf{t}_{ij} \mathbf{d}_j, \qquad \mathbf{d}_i = \begin{pmatrix} P_i^+ \\ P_i^- \end{pmatrix} d_i, \qquad \mathbf{t}_{ij} = \begin{Vmatrix} t_{ij}^{++} & t_{ij}^{+-} \\ t_{ij}^{-+} & t_{ij}^{--} \end{Vmatrix}. \tag{2}$$

The total Hamiltonian of the electronic system with correlated hopping $H = \sum_i H_i + H_t$ includes besides the hopping term H_t that is not local also the single-site contributions H_i. Our aim is to consider the $D \to \infty$ limit and it is convenient to start not from the Dyson equation, that considers the terms with correlated hopping as some kind of many-particle interactions, but from the Larkin equation [6, 7] in coordinate representation

$$\mathbf{G}_{ij}(\omega) = \mathbf{\Xi}_{ij}(\omega) + \sum_{lm} \mathbf{\Xi}_{il}(\omega) \mathbf{t}_{lm} \mathbf{G}_{mj}(\omega), \qquad \mathbf{G}_{\mathbf{k}}(\omega) = \left[\mathbf{\Xi}_{\mathbf{k}}^{-1}(\omega) - \mathbf{t}_{\mathbf{k}} \right]^{-1}, \tag{3}$$

that treats all hopping terms in a same manner. Here, an irreducible part $\mathbf{\Xi}_{ij}(\omega)$, that can not be divided into parts by cutting one hopping line $\mathbf{t}_{lm}$, is introduced.

For the models with correlated hopping all quantities in (3) are matrices and the components of the Green's function $\mathbf{G}_{ij}(\omega)$ are constructed by the projected (Hubbard) operators

$$G_{ij}^{\alpha\gamma}(\omega) = -\left\langle T P_i^\alpha d_i d_j^\dagger P_j^\gamma \right\rangle_\omega = \beta \frac{\delta \Omega}{\delta t_{ji}^{\gamma\alpha}(\omega)}, \qquad \mathbf{G}_{ij}(\omega) = -\left\langle T \mathbf{d}_i \otimes \mathbf{d}_j^\dagger \right\rangle_\omega, \tag{4}$$

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where Ω is the grand canonical potential functional, and the total Green's function is equal

$$G_{ij}(\omega) = -\left\langle T d_i d_j^{\dagger} \right\rangle_{\omega} = \sum_{\alpha\gamma} G_{ij}^{\alpha\gamma}(\omega). \tag{5}$$

In general, the irreducible part $\mathbf{\Xi}_{ij}(\omega)$ is represented diagrammatically by the single-site vertices (because all interactions in H_i are local) connected by hopping lines [5] and in the $D \to \infty$ limit it can be shown (see, e.g. Ref. [4]) that all irreducible parts become local

$$\mathbf{\Xi}_{ij}(\omega) = \delta_{ij}\mathbf{\Xi}(\omega), \quad \mathbf{\Xi}_{\mathbf{k}}(\omega) = \mathbf{\Xi}(\omega). \tag{6}$$

Such matrix representation allows to reformulate the Dynamical Mean-Field Theory of the systems with correlated hopping in terms of local quantities. Indeed, the local irreducible part $\mathbf{\Xi}(\omega)$ depends on the electron hopping only through the local coherent potential $\mathbf{J}(\omega) = \sum_{lm} \mathbf{t}_{ol}\, \mathbf{G}_{lm}^{[o]}(\omega)\, \mathbf{t}_{mo}$, where $\mathbf{G}_{lm}^{[o]}(\omega)$ is the Green's function for the lattice with the removed site o, and it is easy to show that coherent potential $\mathbf{J}(\omega)$ is solution of the following equation

$$\frac{1}{N}\sum_{\mathbf{k}} \left[\mathbf{\Xi}^{-1}(\omega) - \mathbf{t}_{\mathbf{k}}\right]^{-1} = \left[\mathbf{\Xi}^{-1}(\omega) - \mathbf{J}(\omega)\right]^{-1} = \mathbf{G}_{\mathrm{imp}}(\omega) \tag{7}$$

that is the matrix generalization of the known equation (see, e.g. Ref. [2]). Here, $\mathbf{G}_{\mathrm{imp}}(\omega)$ is the Green's function for the effective single-impurity problem with the statistical operator

$$\hat{\rho}_{\mathrm{imp}} = \mathrm{e}^{-\beta H_o} T \exp\left\{ -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' \mathbf{d}_o^{\dagger}(\tau) \mathbf{J}(\tau - \tau') \mathbf{d}_o(\tau') \right\}. \tag{8}$$

Finally, the grand canonical potential for the lattice can be expressed in terms of the grand canonical potential for the impurity model Ω_{imp} by

$$\frac{\Omega_{\mathrm{lat}}}{N} = \Omega_{\mathrm{imp}} - \frac{1}{\beta}\sum_{\nu} \left\{ \frac{1}{N}\sum_{\mathbf{k}} \ln\det\left[1 - \mathbf{\Xi}(i\omega_\nu)\mathbf{t}_{\mathbf{k}}\right] - \ln\det\left[1 - \mathbf{\Xi}(i\omega_\nu)\mathbf{J}(i\omega_\nu)\right] \right\}. \tag{9}$$

Now, let us apply the developed above approach to the Falicov–Kimball model with correlated hopping. The single site Hamiltonian H_i is written

$$H_i = -\mu_f n_{if} - \mu_d n_{id} + U n_{id} n_{if} = -\mu_f P_i^{+} + (U - \mu_d) n_{id} P_i^{+} - \mu_d n_{id} P_i^{-}. \tag{10}$$

Projection operators P_i^{+} and P_i^{-} commute with the total Hamiltonian and the partition function for the impurity is a sum of the partition functions for the subspaces $\alpha = \pm$:

$$Z_{\mathrm{imp}} = \mathrm{Sp}\,\hat{\rho}_{\mathrm{imp}} = \mathrm{e}^{-\beta Q_+} + \mathrm{e}^{-\beta Q_-}, \qquad \Omega_{\mathrm{imp}} = -\frac{1}{\beta}\ln Z_{\mathrm{imp}}, \tag{11}$$

$$Q_\alpha = -\mu_f \delta_{\alpha+} - \frac{1}{\beta}\ln\left(1 + \mathrm{e}^{-\beta(U\delta_{\alpha+} - \mu_d)}\right) - \frac{1}{\beta}\sum_{\nu} \ln\left(1 - \frac{J^{\alpha\alpha}(i\omega_\nu)}{i\omega_\nu + \mu_d - U\delta_{\alpha+}}\right). \tag{12}$$

The Green's functions matrix for the impurity is diagonal ($G_{\mathrm{imp}}^{+-}(\omega) = G_{\mathrm{imp}}^{-+}(\omega) = 0$)

$$G_{\mathrm{imp}}^{++}(\omega) = \frac{\langle P^{+}\rangle}{\omega + \mu_d - U - J^{++}(\omega)}, \qquad G_{\mathrm{imp}}^{--}(\omega) = \frac{\langle P^{-}\rangle}{\omega + \mu_d - J^{--}(\omega)}, \tag{13}$$

and, in addition, we have for the concentrations of the f and d particles

$$n_f = \langle P^{+}\rangle = \frac{1}{Z_{\mathrm{imp}}}\mathrm{e}^{-\beta Q_+}, \qquad n_d = \langle d^{\dagger} d\rangle = \frac{1}{\beta}\sum_{\nu}\left[G_{\mathrm{imp}}^{++}(i\omega_\nu) + G_{\mathrm{imp}}^{--}(i\omega_\nu)\right]. \tag{14}$$

Finally for the Green's function for the lattice we get

$$\begin{aligned}
G^{++}_{\mathbf{k}}(\omega) &= \frac{1}{\mathcal{D}_{\mathbf{k}}(\omega)}\left[\omega+\mu_d - J^{--}(\omega)\langle P^+\rangle - t^{--}_{\mathbf{k}}\langle P^-\rangle\right]\langle P^+\rangle,\\
G^{--}_{\mathbf{k}}(\omega) &= \frac{1}{\mathcal{D}_{\mathbf{k}}(\omega)}\left[\omega+\mu_d - U - J^{++}(\omega)\langle P^-\rangle - t^{++}_{\mathbf{k}}\langle P^+\rangle\right]\langle P^-\rangle,\\
G^{+-(-+)}_{\mathbf{k}}(\omega) &= -\frac{1}{\mathcal{D}_{\mathbf{k}}(\omega)}\left[J^{+-(-+)}(\omega) - t^{+-(-+)}_{\mathbf{k}}\right]\langle P^+\rangle\langle P^-\rangle,\\
\mathcal{D}_{\mathbf{k}}(\omega) &= \left[\omega+\mu_d - J^{--}(\omega)\langle P^+\rangle - t^{--}_{\mathbf{k}}\langle P^-\rangle\right]\\
&\quad\times\left[\omega+\mu_d - U - J^{++}(\omega)\langle P^-\rangle - t^{++}_{\mathbf{k}}\langle P^+\rangle\right]\\
&\quad-\left[J^{+-}(\omega) - t^{+-}_{\mathbf{k}}\right]\left[J^{-+}(\omega) - t^{-+}_{\mathbf{k}}\right]\langle P^+\rangle\langle P^-\rangle.
\end{aligned} \tag{15}$$

Now, the total Green's function (5) for the Falicov–Kimball model with correlated hopping can be written in the Dyson representation as $G_{\mathbf{k}}(\omega) = [\omega+\mu_d-\Sigma_{\mathbf{k}}(\omega)-\bar{t}_{\mathbf{k}}]^{-1}$, where $\bar{t}_{\mathbf{k}} = t^{++}_{\mathbf{k}}\langle P^+\rangle^2 + t^{--}_{\mathbf{k}}\langle P^-\rangle^2 + \left(t^{+-}_{\mathbf{k}}+t^{-+}_{\mathbf{k}}\right)\langle P^+\rangle\langle P^-\rangle$ is the Hartree renormalized (mean-field) hopping already introduced by Schiller [3] and

$$\Sigma_{\mathbf{k}}(\omega) = U\langle P^+\rangle + J_3(\omega)\langle P^+\rangle\langle P^-\rangle + \frac{U_{1\mathbf{k}}(\omega)U_{2\mathbf{k}}(\omega)\langle P^+\rangle\langle P^-\rangle}{\omega+\mu_d - U\langle P^-\rangle - \bar{J}(\omega) - t_{3\mathbf{k}}\langle P^+\rangle\langle P^-\rangle} \tag{16}$$

is the momentum dependent (non local) self-energy. Here

$$\begin{aligned}
U_{1(2)\mathbf{k}}(\omega) &= U + \left[t^{++}_{\mathbf{k}} - t^{-+(+-)}_{\mathbf{k}} - J^{--}(\omega) + J^{-+(+-)}(\omega)\right]\langle P^+\rangle\\
&\quad+\left[t^{+-(-+)}_{\mathbf{k}} - t^{--}_{\mathbf{k}} - J^{+-(-+)}(\omega) + J^{++}(\omega)\right]\langle P^-\rangle
\end{aligned} \tag{17}$$

describes the renormalization of the interaction U and

$$\begin{aligned}
\bar{J}(\omega) &= J^{++}(\omega)\langle P^-\rangle^2 + J^{--}(\omega)\langle P^+\rangle^2 + \left(J^{+-}(\omega)+J^{-+}(\omega)\right)\langle P^+\rangle\langle P^-\rangle,\\
J_3(\omega) &= J^{++}(\omega) + J^{--}(\omega) - J^{+-}(\omega) - J^{-+}(\omega),\\
t_{3\mathbf{k}} &= t^{++}_{\mathbf{k}} + t^{--}_{\mathbf{k}} - t^{+-}_{\mathbf{k}} - t^{-+}_{\mathbf{k}}.
\end{aligned} \tag{18}$$

In his article Schiller [3] considered the case of $t_{3\mathbf{k}} = 0$ and from (16) we get the same result for the self-energy $\Sigma_{\mathbf{k}}(\omega) = \Sigma_0(\omega) + \Sigma_1(\omega)t_{\mathbf{k}} + \Sigma_2(\omega)t^2_{\mathbf{k}}$ that for the nearest-neighbor hopping $t_{\mathbf{k}}$ it contains only local, nearest-neighbor and next-nearest-neighbor contributions. But in the general case of $t_{3\mathbf{k}} \neq 0$ the self-energy "spreads" over all lattice.

Now, let us consider some limiting cases. At half filling $\mu_d = \mu_f$, $n_f + n_d = 1$, the spectral weight function is symmetric for two points [3]. One of them correspond to the absence of correlated hopping ($t^{\alpha\gamma} = t$). Another symmetric point $t_2/t_1 = -1$, $t_3 = 0$ ($t^{--} = t_1$, $t^{+-} = t^{-+} = t_1+t_2$, $t^{++} = t_1+2t_2+t_3$) was considered for the 1D Hubbard model when exact results can be obtained [8]. In Ref. [9] it was shown that in this case the direct transition from the superconducting state to the Mott insulator takes place. This symmetric point corresponds to the case of the diagonal hopping matrix $t^{--}_{\mathbf{k}} = -t^{++}_{\mathbf{k}} = t_{\mathbf{k}}$, $t^{+-}_{\mathbf{k}} = t^{-+}_{\mathbf{k}} = 0$ when hopping is allowed only between the sites with the same occupancy. Now, for the Falicov–Kimball model the coherent potential matrix is also diagonal ($J^{+-}(\omega) = J^{-+}(\omega) = 0$) and for the semi-elliptic density of states of the half-width W we have ($\alpha = \pm$)

$$J^{\alpha\alpha}(\omega) = \frac{W^2}{4}G^{\alpha\alpha}(\omega) = \frac{1}{2}\left(\omega+\mu_d - U\delta_{\alpha+}\right) + \frac{i}{2}\sqrt{W^2_\alpha - \left(\omega+\mu_d-U\delta_{\alpha+}\right)^2}, \tag{19}$$

where $W_{\pm}^2 = W^2\langle P^{\pm}\rangle$. The spectral weight function contains two bands

$$\rho(\omega) = \frac{1}{\pi}\,\mathrm{Im}\,G_{\mathrm{imp}}(\omega - i0^+) = \frac{2\langle P^+\rangle}{\pi W_+^2}\sqrt{W_+^2 - (\omega - U)^2} + \frac{2\langle P^-\rangle}{\pi W_-^2}\sqrt{W_-^2 - \omega^2}, \quad (20)$$

separated by the gap $\Delta = U - W_+ - W_- = U - W\left(\sqrt{\langle P^+\rangle} + \sqrt{\langle P^-\rangle}\right)$ that is temperature dependent out of half filling and at half-filling, when $n_f = n_d = \frac{1}{2}$, it disappears at $U_c = W\sqrt{2}$ (the Mott transition point).

Out of these symmetric points the Falicov–Kimball model with correlated hopping possess the temperature driven Mott transition (see Fig. 1).

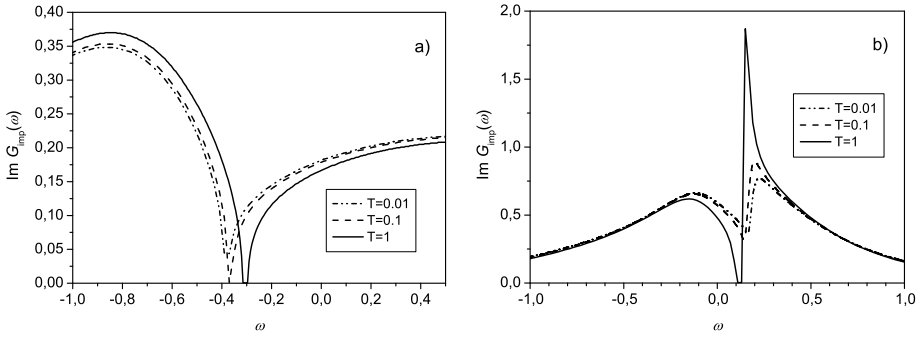

Figure 1: Temperature development of the gap (Mott transition) for $t_2/t_1 = 0.5$, $U = 1.7$ (a) and $t_2/t_1 = -0.5$, $U = 0.3$ (b) for the $D = \infty$ hypercubic lattice with nearest neighbor hopping at half filling $\mu_d = \mu_f$, $n_f + n_d = 1$

In this article we presented the general approach to the description of the correlated hopping in the Dynamical Mean-Field Theory. It is based on the Larkin equation (expansion over electron hopping around the atomic limit) that considers all hopping terms, including correlated hopping, in a same manner. Another starting point is the local character of the irreducible part (irreducible cumulant) of the Green's functions constructed by the projected (Hubbard) operators in the $D \to \infty$ limit that is more general statement then the local character of the self-energy which in the case of correlated hopping is unlocal. Such approach keeps the Dynamical Mean-Field Theory local ideology and allows to calculate the thermodynamical functions. As an example the Falicov-Kimball model with correlated hopping and its limit case are considered when exact results can be obtained. In particular, the temperature driven Mott transition in the Falicov–Kimball model with correlated hopping is investigated.

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